

**Effect of on-site Coulomb repulsion on superconductivity in the boson-fermion model**

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(Received 22 February 2002; published 10 October 2002)

We study the influence of the repulsive Coulomb interactions on the thermodynamic properties of the boson-fermion model with an anisotropic ( $d$ -wave and extended  $s$ -wave) order parameter. Superconductivity is induced in this model from the anisotropic charge exchange interaction between the conduction-band fermions (electrons or holes) and the immobile hard-core bosons (the localized electron pairs). The on-site Coulomb repulsion competes with this pairing interaction and hence is expected to have a detrimental influence on superconductivity. We analyze this effect in some detail, considering the two opposite limits of the weak and strong repulsion. A possible crossover between both these regimes is also discussed.

DOI: 10.1103/PhysRevB.66.134512

PACS number(s): 74.20.-z, 74.20.Mn, 74.20.Rp, 74.25.Dw

**I. INTRODUCTION**

The boson-fermion (BF) model describes a mixture of the narrow-band fermions coupled to a system of the composite hard-core bosons. Initially, this type of an effective Hamiltonian was invented for a system of itinerant electrons interacting with local lattice deformations in the crossover regime between adiabatic and antiadiabatic limits.<sup>1</sup> Later, the same model was independently considered by a number of authors<sup>2-5</sup> as a possible scenario for a mechanism of high-temperature superconductivity (HTSC). There have also been attempts to apply a similar BF model to explain certain aspects of the Bose-condensed atoms of alkali metals.<sup>6</sup>

This model reveals a rich physics both in its normal phase and the broken symmetry superconducting-superfluid states. As shown in mean-field-type studies<sup>3,5</sup> there is a characteristic temperature  $T_c$  below which fermions are driven to the superconducting phase and simultaneously bosons start to Bose condense. This result has been confirmed (neglecting the hard-core nature of bosons) by means of the shielded potential approximation<sup>7</sup> and with the help of the renormalization group approach.<sup>8</sup> Moreover, when approaching the critical temperature from above, the pairwise correlations start to manifest themselves strongly. In particular, they may give rise to the formation of a pseudogap in the fermion spectrum. This effect, known experimentally from a variety of measurements (see, e.g., the review in Ref. 9), provides a firm argument for the application of this model to describe HTSC materials.

Pseudogap formation and its variation with a lowering temperature have been carefully investigated for the BF model using (a) the self-consistent perturbative treatment of the boson-fermion coupling,<sup>10,11</sup> (b) the perturbative treatment of the kinetic processes (in the manner of Hubbard I for the fermion hopping) with respect to the exact solution of this model in its atomic limit,<sup>12</sup> (c) the dynamical mean-field theory (DMFT) equations which have been self-consistently solved within the noncrossing approximation for the auxiliary impurity problem,<sup>13</sup> and (d) the renormalization group technique.<sup>8</sup>

Many experimental data, especially angle-resolved photoemission spectroscopy,<sup>14</sup> seem to suggest the anisotropic  $d$ -wave type structure of both: the pseudogap and true super-

conducting gap. However, there are also known some measurements—for instance the  $c$ -axis Josephson tunneling<sup>15</sup> and the photoemission spectroscopy on  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$  (Ref. 16)—which provide strong arguments for a nonzero  $s$ -wave ingredient of the order parameter. In a most realistic situation one can expect that the order parameter of the HTSC cuprates acquires a mixed  $s+d$  or  $s+id$  symmetry. The possibility for the appearance of the mixed symmetry superconducting phase has been theoretically explored on quite general grounds using a two-dimensional electron system with anisotropic potential  $V = V_s + V_d$  of arbitrary (from weak to strong) attraction strength.<sup>17</sup> So far, most studies of the superconductivity within the BF model have been performed for the isotropic pairing interaction. Some attempts to analyze the  $d$ -pairing superconductivity together with a microscopic justification for introducing the BF-type Hamiltonian can be found in the paper by Geshkenbein *et al.*<sup>18</sup> Very recently, a more formal way has been explored by Micnas *et al.*<sup>19</sup>

In this paper we shall investigate various kinds of superconducting phases induced by an anisotropic potential of the BF model in the presence of Coulomb interactions between fermions. For simplicity we shall concentrate only on the case of on-site repulsion  $U > 0$ , where  $U = \langle ii | (e^2/|r|) | ii \rangle$  in the Wannier representation. In general, one expects that the on-site repulsion (which prevents fermions from forming local pairs) would compete with the correlations induced by the boson-fermion coupling (this interaction is a driving force for the pairing in the BF model and is responsible for inducing the pseudogap at temperatures  $T^* > T > T_c$  and the true superconducting gap when  $T \leq T_c$ ). We shall address the following question: what is the extent of the detrimental influence of  $U$  on the pairing correlations?

The above-mentioned competition has been already studied in a normal phase of the BF model using the nonperturbative approach of the DMFT.<sup>20</sup> In our paper we shall investigate the anisotropic superconducting phase. To make our study feasible we assume that the pairing interactions are relatively weak (the meaning of this assumption is explained in the next section) and we try to estimate the influence of the Coulomb repulsion varying its intensity from the weak-to strong-interaction limit.

## II. MODEL

The Hamiltonian of the system under consideration consists of the two parts  $H = H^{BF} + H^{Coul}$ . The first of them refers to the standard BF model Hamiltonian<sup>5</sup>

$$H^{BF} = \sum_{\mathbf{k}, \sigma} (\varepsilon_{\mathbf{k}} - \mu) c_{\mathbf{k}, \sigma}^{\dagger} c_{\mathbf{k}, \sigma} + (\Delta_B - 2\mu) \sum_i b_i^{\dagger} b_i + \frac{1}{\sqrt{N}} \sum_{\mathbf{k}, \mathbf{q}} (v_{\mathbf{k}, \mathbf{q}} b_{\mathbf{q}}^{\dagger} c_{-\mathbf{k} + \mathbf{q}/2, \downarrow} c_{\mathbf{k} + \mathbf{q}/2, \uparrow} + \text{H.c.}), \quad (1)$$

and the second part denotes the on-site interaction between fermions  $H^{Coul} = U \sum_i n_{i, \downarrow} n_{i, \uparrow}$ . We use here the standard notation for the annihilation (creation) operators of fermions,  $c_{i, \sigma}$  ( $c_{i, \sigma}^{\dagger}$ ), with spin  $\sigma$  and for the hard-core boson  $b_i$  ( $b_i^{\dagger}$ ) at site  $i$  of the two-dimensional square lattice. The indices  $\mathbf{k}$  and  $\mathbf{q}$  in Eq. (1) denote the coordinates of momentum space. We assume the tight-binding dispersion for fermions,  $\varepsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y)$ , and set the bandwidth  $D = 8t$  as a unit ( $D \equiv 1$ ).

It is important to remark now that we let the boson-fermion exchange potential  $v_{\mathbf{k}, \mathbf{q}}$  to be anisotropic. As explained in Ref. 18 the low-energy physics of this model is dominated by bosons of small momenta  $|\mathbf{q}| \approx 0$ . Usually, the magnitudes of the superconducting gap in HTSC materials are of the order of several meV (which is  $\sim 10^{-3}$  of the bandwidth  $D$ ). It is thus reasonable to assume that the pairing potential  $v_{\mathbf{k}, \mathbf{q}}$ , which establishes the energy scale for  $T_c$  and  $\Delta_{sc}(T=0)$ , is small as compared to  $D$ . In such a case the following mean-field decoupling is justified:

$$\sum_{\mathbf{q}} v_{\mathbf{k}, \mathbf{q}} b_{\mathbf{q}}^{\dagger} c_{-\mathbf{k} + \mathbf{q}/2, \downarrow} c_{\mathbf{k} + \mathbf{q}/2, \uparrow} \approx v_{\mathbf{k}, \mathbf{q}=\mathbf{0}} (\langle b_{\mathbf{q}=\mathbf{0}} \rangle)^* c_{-\mathbf{k}, \downarrow} c_{\mathbf{k}, \uparrow} + b_{\mathbf{q}=\mathbf{0}}^{\dagger} \langle c_{-\mathbf{k}, \downarrow} c_{\mathbf{k}, \uparrow} \rangle. \quad (2)$$

We further write down the anisotropic potential  $v_{\mathbf{k}, \mathbf{0}}$  as a product:<sup>19</sup>

$$v_{\mathbf{k}, \mathbf{0}} \equiv g \phi_{\mathbf{k}}, \quad (3)$$

where  $g$  characterizes the interaction strength and  $\phi_{\mathbf{k}}$  stands for the dimensionless factor which has to reflect the fourfold symmetry of  $\text{CuO}_2$  planes of the HTSC cuprates. In general the anisotropy factor  $\phi_{\mathbf{k}}$  can be represented as

$$\phi_{\mathbf{k}} = \alpha_0 + \alpha_s (\cos k_x + \cos k_y) + \alpha_d (\cos k_x - \cos k_y) \quad (4)$$

and the coefficients  $\alpha_{0,s,d}$  denote a relative contribution of the isotropic, the extended  $s$ -wave, and the  $d$ -wave parts into the order parameter of the superconducting phase. They should be adjusted depending on the specific material. If, for example,  $\alpha_0 \neq 0$  and  $\alpha_d \neq 0$ , we would have the order parameter of a mixed  $s+d$  or  $s+id$  symmetry. Since our main interest is focused on the competition between the Coulomb interaction and the superconductivity, we further consider for clarity only the pure extended  $s$ - or  $d$ -wave symmetries when  $\phi_{\mathbf{k}} = \cos k_x \pm \cos k_y$ .

After the mean-field decoupling for the boson-fermion interaction (2) we are left with an effective Hamiltonian composed of the separated fermion and boson contributions<sup>1</sup>  $H \approx H^F + H^B$ :

$$H^F = \sum_{\mathbf{k}, \sigma} \xi_{\mathbf{k}} c_{\mathbf{k}, \sigma}^{\dagger} c_{\mathbf{k}, \sigma} + U \sum_i n_{i, \downarrow} n_{i, \uparrow} + \sum_{\mathbf{k}} (g \rho \phi_{\mathbf{k}} c_{\mathbf{k}, \uparrow}^{\dagger} c_{-\mathbf{k}, \downarrow}^{\dagger} + \text{H.c.}), \quad (5)$$

$$H^B = \sum_i (E_0 b_i^{\dagger} b_i + g x b_i^{\dagger} + g x^* b_i). \quad (6)$$

We introduced here the abbreviations for energies measured from the chemical potential  $\xi_{\mathbf{k}} = \varepsilon_{\mathbf{k}} - \mu$ ,  $E_0 = \Delta_B - 2\mu$  and for the two order parameters  $x = \sum_{\mathbf{k}} \phi_{\mathbf{k}} \langle c_{-\mathbf{k}, \downarrow} c_{\mathbf{k}, \uparrow} \rangle$ ,  $\rho = \langle b_{\mathbf{q}=\mathbf{0}} \rangle / \sqrt{N} = \langle b_i \rangle$ .

We can easily solve the hard-core boson part of the problem. For a given site  $i$  one finds the true eigenstates using the unitary transformation

$$|A\rangle_i = \cos(\alpha) |0\rangle_i + \sin(\alpha) |1\rangle_i, \quad (7)$$

$$|B\rangle_i = -\sin(\alpha) |0\rangle_i + \cos(\alpha) |1\rangle_i, \quad (8)$$

such that  $\tan(2\alpha) = (-2gx)/E_0$ , where  $|0\rangle_i$  and  $|1\rangle_i$  refer correspondingly to the empty and singly occupied (by the hard-core boson) site  $i$ . In a straightforward calculation we can determine the expectation values for the number operator  $n^B = \sum_i \langle b_i^{\dagger} b_i \rangle$  and for the order parameter  $\rho$ ,<sup>5,19</sup>

$$n^B = \frac{1}{2} - \frac{E_0}{4\gamma} \tanh\left(\frac{\gamma}{k_B T}\right), \quad (9)$$

$$\rho = -\frac{gx}{2\gamma} \tanh\left(\frac{\gamma}{k_B T}\right), \quad (10)$$

where  $\gamma = \sqrt{(E_0/2)^2 + |gx|^2}$  and  $k_B$  is the Boltzmann constant.

## III. WEAK-INTERACTION LIMIT

First, we consider the weak-coupling limit when  $U$  is fairly smaller than  $D$ . We are in a position to utilize then the Hartree-Fock-Gorkov linearization for the on-site interaction  $n_{i, \downarrow} n_{i, \uparrow} \approx n_{i, \downarrow} \langle n_{i, \uparrow} \rangle + \langle n_{i, \downarrow} \rangle n_{i, \uparrow} + \langle c_{i, \downarrow}^{\dagger} c_{i, \downarrow}^{\dagger} \rangle c_{i, \downarrow} c_{i, \uparrow} + c_{i, \uparrow}^{\dagger} c_{i, \uparrow}^{\dagger} \langle c_{i, \downarrow} c_{i, \downarrow} \rangle$ . The Hamiltonian of the fermion subsystem (5) reduces then simply to the BCS structure  $H^F \approx \sum_{\mathbf{k}, \sigma} \tilde{\xi}_{\mathbf{k}} c_{\mathbf{k}, \sigma}^{\dagger} c_{\mathbf{k}, \sigma} + \sum_{\mathbf{k}} (\Delta_{\mathbf{k}}^{(eff)} c_{\mathbf{k}, \uparrow}^{\dagger} c_{-\mathbf{k}, \downarrow}^{\dagger} + \text{H.c.})$  with  $\tilde{\xi}_{\mathbf{k}} = \xi_{\mathbf{k}} + U n^F/2$  (we assume a paramagnetic state  $\langle n_{i, \uparrow} \rangle = \langle n_{i, \downarrow} \rangle \equiv n^F/2$ ). A role of the effective gap parameter is played here by

$$\Delta_{\mathbf{k}}^{(eff)} = \Delta_0 + g \rho \phi_{\mathbf{k}}, \quad (11)$$

where the isotropic part is given by  $\Delta_0 = U \langle c_{i, \downarrow} c_{i, \uparrow} \rangle$ . Standard methods of the solid-state theory give the following equations for expectation values:

$$n^F = 1 - \sum_{\mathbf{k}} \frac{\tilde{\xi}_{\mathbf{k}}}{E_{\mathbf{k}}} \tanh\left(\frac{E_{\mathbf{k}}}{2k_B T}\right), \quad (12)$$

$$\langle c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} \rangle = \frac{-\Delta_{\mathbf{k}}^{(eff)}}{2E_{\mathbf{k}}} \tanh\left(\frac{E_{\mathbf{k}}}{2k_B T}\right), \quad (13)$$

with a typical gapped spectrum  $E_{\mathbf{k}} = \sqrt{\tilde{\xi}_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}^{(eff)}|^2}$  in the superconducting phase.

It is worth mentioning that in a case of  $d$  pairing (i.e., for  $\phi_{\mathbf{k}} = \cos k_x - \cos k_y \equiv \eta_{\mathbf{k}}$ ) the isotropic component  $\Delta_0$  of the gap parameter (11) does identically vanish. To prove this let us substitute Eq. (13) into the definition of  $\Delta_0 = U \sum_{\mathbf{k}} \langle c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} \rangle$  to obtain

$$\Delta_0 = -U \sum_{\mathbf{k}} \frac{\Delta_0 + g \rho \eta_{\mathbf{k}}}{2E_{\mathbf{k}}} \tanh\left(\frac{E_{\mathbf{k}}}{2k_B T}\right). \quad (14)$$

Since integration over the Brillouin zone of the part containing  $\eta_{\mathbf{k}}$  gives zero, so, for  $U > 0$ , Eq. (14) has the only possible solution  $\Delta_0 = 0$ . It is not surprising because the repulsive interactions by themselves are not able to induce the on-site fermion pairs.

If the boson fermion potential (3) is isotropic or takes a form of the  $s$  wave ( $\phi_{\mathbf{k}} = \cos k_x + \cos k_y$ ), then in general  $\Delta_0 \neq 0$ . From a consideration similar to the one discussed above [Eq. (14) is valid except that  $\eta_{\mathbf{k}}$  should be replaced by  $\phi_{\mathbf{k}}$ ] we can determine a relative ratio  $\Delta_0/g\rho$ . The extended  $s$ -wave gap parameter is now given by

$$\Delta_{\mathbf{k}}^{(eff)} = g \rho \left( \phi_{\mathbf{k}} - \frac{\sum_{\mathbf{k}} (U \phi_{\mathbf{k}}/2E_{\mathbf{k}}) \tanh(E_{\mathbf{k}}/2k_B T)}{1 + \sum_{\mathbf{k}} (U/2E_{\mathbf{k}}) \tanh(E_{\mathbf{k}}/2k_B T)} \right). \quad (15)$$

For the isotropic boson fermion potential ( $\phi_{\mathbf{k}} = 1$ ), Eq. (15) simplifies further to give a  $\mathbf{k}$ -independent gap  $\Delta^{(eff)} = g \rho [1 + \sum_{\mathbf{k}} (U/2E_{\mathbf{k}}) \tanh(E_{\mathbf{k}}/2k_B T)]^{-1} < g \rho$ . This expression explicitly shows a detrimental role of the on-site repulsion on the isotropic superconducting phase. Such a problem has been previously addressed<sup>7,21</sup> neglecting the hard-core nature of bosons and using the random phase approximation (RPA) treatment for the Coulomb repulsion.

#### IV. STRONG-INTERACTION LIMIT

In a case of the strong interactions ( $U > D$ ) we make use of the slave-boson technique proposed by Kotliar and Ruckenstein.<sup>22</sup> For simplicity we shall consider here only the extreme limit  $U \rightarrow \infty$ .

We represent the fermion operators as  $c_{i,\sigma} = a_i^\dagger f_{i,\sigma}$  and  $c_{i,\sigma}^\dagger = f_{i,\sigma}^\dagger a_i$ , where the auxiliary boson operator  $a_i$  ( $a_i^\dagger$ ) refers to the annihilation (creation) of the empty state at site  $i$  and fermion operator  $f_{i,\sigma}$  ( $f_{i,\sigma}^\dagger$ ) corresponds to annihilation (creation) of the singly occupied site  $i$  with spin  $\sigma$ . No double occupancy is allowed and this can be formally expressed via the local constraint  $a_i^\dagger a_i + \sum_{\sigma} f_{i,\sigma}^\dagger f_{i,\sigma} = 1$ .

Using the real-space (Wannier states) representation we

can rewrite the Hamiltonian (5) in terms of the new operators as

$$\begin{aligned} H^F = & \sum_{i,j,\sigma} t_{i,j} f_{i,\sigma}^\dagger a_i a_j^\dagger f_{j,\sigma} - \mu \sum_{i,\sigma} f_{i,\sigma}^\dagger f_{i,\sigma} \\ & + \left( \rho \sum_{i,j} V_{i,j} f_{i,\uparrow}^\dagger a_i a_j^\dagger f_{j,\downarrow} + \text{H.c.} \right) \\ & + \sum_i \lambda_i \left( a_i^\dagger a_i + \sum_{\sigma} f_{i,\sigma}^\dagger f_{i,\sigma} - 1 \right). \end{aligned} \quad (16)$$

We used here the identity  $a_i a_i^\dagger = 1$ ,<sup>22</sup> and the last term takes account of the local constraint ( $\lambda_i$  stands for the Lagrange multiplier).  $V_{i,j}$  is the exchange potential whose Fourier transform is given by Eq. (3) and, as usual,  $t_{i,j}$  denotes the hopping integral.

Next, we approximate Eq. (16) by (i) replacing the slave-boson operators by their expectation values which are assumed to be site independent  $a_i \approx \langle a_i \rangle \approx r$  and (ii) replacing the local multipliers by the global one  $\lambda_i \approx \lambda$ . In this (mean-field) approximation for the slave bosons one obtains

$$\begin{aligned} H^F \approx & \sum_{\mathbf{k},\sigma} (r^2 \varepsilon_{\mathbf{k}} - \mu + \lambda) f_{\mathbf{k},\sigma}^\dagger f_{\mathbf{k},\sigma} \\ & + \sum_{\mathbf{k}} (r^2 g \rho \phi_{\mathbf{k}} f_{\mathbf{k},\uparrow}^\dagger f_{-\mathbf{k},\downarrow}^\dagger + \text{H.c.}). \end{aligned} \quad (17)$$

The global parameters  $\lambda$ ,  $r$  are determined from a minimization of the total energy  $\langle H \rangle$ . This criterion leads to

$$r^2 = 1 - n^F, \quad (18)$$

$$\lambda = - \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} \langle f_{\mathbf{k},\sigma}^\dagger f_{\mathbf{k},\sigma} \rangle - 2 \text{Re} \left\{ g \rho^* \sum_{\mathbf{k}} \phi_{\mathbf{k}} \langle f_{-\mathbf{k},\downarrow} f_{\mathbf{k},\uparrow} \rangle \right\}. \quad (19)$$

As can be noticed from Eq. (17), the Hamiltonian of the fermion subsystem  $H^F$  is again reduced to the BCS structure. We thus have the same solution for the expectation values as given in Eqs. (12) and (13) with a difference that now

$$\tilde{\xi}_{\mathbf{k}} = r^2 \varepsilon_{\mathbf{k}} - \mu + \lambda, \quad (20)$$

$$\Delta_{\mathbf{k}} = r^2 g \rho \phi_{\mathbf{k}}. \quad (21)$$

Both the effective fermion bandwidth  $D^{(eff)} = r^2 D$  and the effective pairing potential  $V_{\mathbf{k}}^{(eff)} = r^2 g \phi_{\mathbf{k}}$  reduce down to zero when fermion occupation approaches the half-filling. Under such circumstances the system is driven into the Mott insulating state.

#### V. CROSSOVER

Finally we consider here a regime of the intermediate  $U$  for which we adopt the procedure used earlier by us<sup>23</sup> in the context of the extended Hubbard model. We introduce the Nambu representation  $\Psi_{\mathbf{k}}^\dagger = (c_{\mathbf{k},\uparrow}^\dagger c_{-\mathbf{k},\downarrow})$ ,  $\Psi_{\mathbf{k}} = (\Psi_{\mathbf{k}}^\dagger)^\dagger$  and, as a first step, determine the unperturbed Green's function

$G^0(\mathbf{k}, \omega) = \langle\langle \Psi_{\mathbf{k}}; \Psi_{\mathbf{k}}^\dagger \rangle\rangle_\omega$  neglecting the interaction  $U$  in the fermion Hamiltonian (5):

$$\begin{bmatrix} i\omega_n - \xi_{\mathbf{k}} & -g\rho^* \phi_{\mathbf{k}} \\ -g\rho \phi_{\mathbf{k}} & i\omega_n - \xi_{\mathbf{k}} \end{bmatrix} G_0(\mathbf{k}, i\omega_n) = \mathbf{1}. \quad (22)$$

Next, we compute the dressed Green's function using the matrix Dyson equation

$$G^{-1}(\mathbf{k}, i\omega_n) = G_0^{-1}(\mathbf{k}, i\omega_n) - \Sigma(\mathbf{k}, i\omega_n). \quad (23)$$

In order to proceed we simplify the self-energy matrix by the following ansatz:<sup>23</sup>

$$\Sigma(\mathbf{k}, i\omega_n) \simeq \begin{bmatrix} \Sigma_N(\mathbf{k}, i\omega_n) & U \langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \rangle \\ U \langle c_{i\downarrow} c_{i\uparrow} \rangle & -\Sigma_N(\mathbf{k}, -i\omega_n) \end{bmatrix}. \quad (24)$$

Without specifying the diagonal elements of Eq. (24) we denote  $\Sigma_{11}(\mathbf{k}, i\omega_n)$  by  $\Sigma_N(\mathbf{k}, i\omega_n)$  and make use of the identity  $\Sigma_{22}(\mathbf{k}, i\omega_n) = -\Sigma_{11}(\mathbf{k}, -i\omega_n)$ . The off-diagonal elements are approximated by us by a contribution corresponding to the result deduced from the mean-field-type theory discussed in Sec. III. The channel of the superconducting correlations is treated by us in Eq. (24) approximately.

If one knew  $\Sigma_N(\mathbf{k}, i\omega_n)$ , then the needed expectation values can be found according to the standard field theoretical relation  $\langle AB \rangle = \beta^{-1} \sum_{n=-\infty}^{\infty} \langle\langle B; A \rangle\rangle_{i\omega_n}$ , where  $\beta = 1/k_B T$ . In particular, we obtain<sup>23</sup>

$$\langle c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\uparrow} \rangle = \beta^{-1} \sum_n \frac{i\omega_n + \xi_{\mathbf{k}} + \Sigma_N(-i\omega_n)}{|i\omega_n - \xi_{\mathbf{k}} - \Sigma_N(i\omega_n)|^2 + |\Delta_{\mathbf{k}}^{(eff)}|^2}, \quad (25)$$

$$\langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle = \beta^{-1} \sum_n \frac{\Delta_{\mathbf{k}}^{(eff)}}{|i\omega_n - \xi_{\mathbf{k}} - \Sigma_N(i\omega_n)|^2 + |\Delta_{\mathbf{k}}^{(eff)}|^2}, \quad (26)$$

where again  $\Delta_{\mathbf{k}}^{(eff)}$  is given by Eq. (11).

It is worth noticing that  $\Sigma_N(\mathbf{k}, i\omega_n)$  has the meaning of the normal phase self-energy for the standard Hubbard model. Of course there is no exact solution for  $\Sigma_N$  available so far except maybe from numerical exact diagonalization or quantum Monte Carlo studies. However, depending on the magnitude of the on-site interaction, one can use various approximate estimations. Let us point out a few possibilities.

Starting from the weak-interaction limit the simplest substitution for  $\Sigma_N$  is the mean-field value  $Un^F/2$  as discussed in Sec. III. With an increase of  $U$  one can proceed by including some higher-order corrections, like, for example, of the second order in  $U$ .<sup>24</sup> Going toward the Mott transition regime  $U = U_{cr} \sim D$  (for the half-filled fermion system) one could work, for example, with the so-called alloy analogy approximation (AAA).<sup>23</sup> In a more subtle way one could estimate the momentum-independent self-energy  $\Sigma_N(\omega)$  by adopting the dynamical mean-field theory (which becomes exact in the limit of infinite spatial dimensions). The strong interaction case can be described in a satisfactory way either with

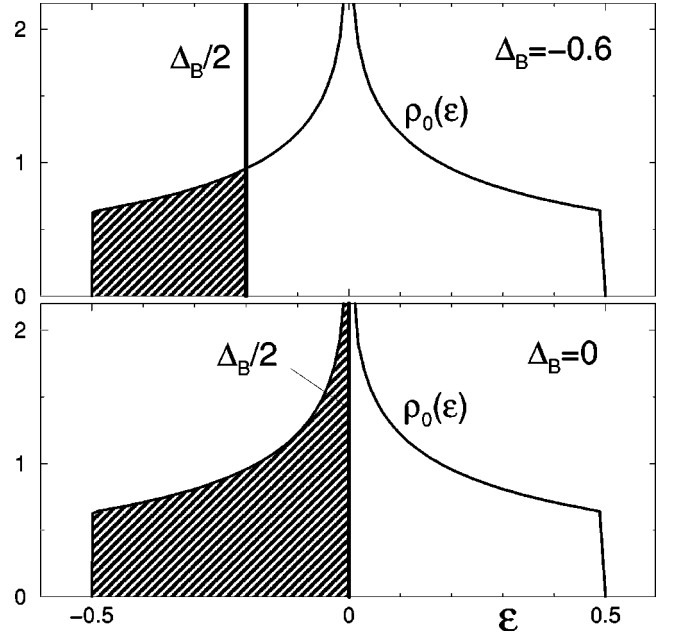


FIG. 1. A schematic illustration of the two distinct critical fermion concentrations: (top)  $n_F \simeq 0.4$  when the boson energy  $\Delta_B/2 = -0.3$  and (bottom)  $n_F = 1$  when  $\Delta_B/2 = 0$ . The shaded areas show the occupied fermion states at zero temperature.

the AAA, DMFT, or simple Hubbard I approximation. Here we apply the AAA procedure to study a regime near the Mott transition.

## VI. NUMERICAL RESULTS

As far as the Coulomb repulsion is concerned we expect that its effectiveness should strongly depend on the concentration of fermions. In the regime of small fermion concentration (dilute limit) this interaction should not be very efficient and, in particular, it would not affect the superconducting-type correlations induced by the boson-fermion exchange. On the other hand, we expect that the strongest effects of the on-site Coulomb repulsion might appear for a system with a nearly half-filled fermion system  $n_F = 1$ .

In absence of the Coulomb interactions, the superconducting phase (isotropic or anisotropic one) of the BF model is formed when the fermion concentration is properly adjusted. The Fermi energy  $\epsilon_F$  must be close enough to the boson level because only then can the charge exchange between the hard-core bosons and fermion pairs induce long-range coherence.<sup>25</sup> So the needed concentration of fermions is roughly given by  $n_F = 2 \int_{-D/2}^{\epsilon_F = \Delta_B/2} \rho_0(\epsilon) d\epsilon$ , where  $\rho_0(\epsilon)$  denotes the density of states of the free (noninteracting) fermion system.

In this section we present results obtained numerically for the BF model in the two distinct cases when the critical fermion concentration is (a) small, which takes place when  $\Delta_B/2$  lies far aside the center of fermion band, and (b) close to half-filling, when  $\Delta_B/2$  is located in the center of fermion band. We thus choose the two values  $\Delta_B/2 = -0.3$  and  $0$ ; see Fig. 1.

We take the boson fermion potential  $g = 0.1$  in all the

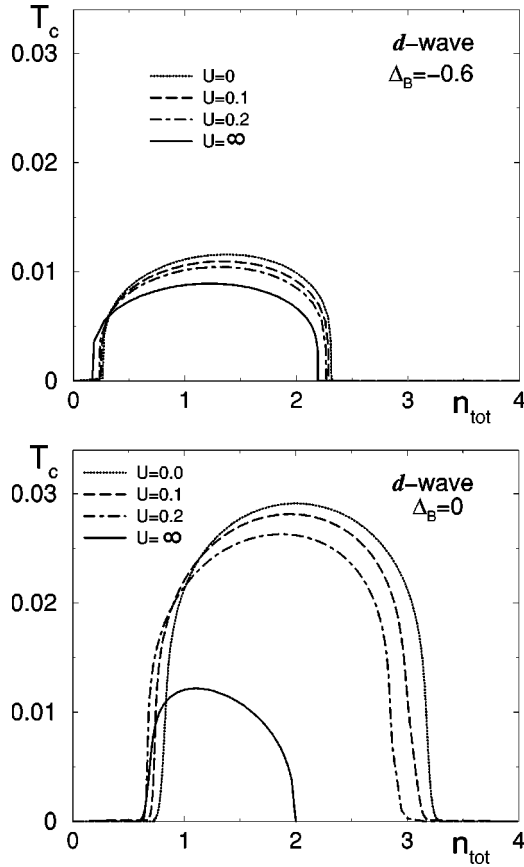


FIG. 2. Transition temperature  $T_c$  into the  $d$ -wave superconducting phase as a function of the total concentration  $n_{tot}$  for the two representative boson level values  $\Delta_B = -0.6$  (top) and  $\Delta_B = 0$  (bottom). Curves corresponding to  $U = 0.1$  and  $0.2$  were obtained from the mean-field approximation, while  $U = \infty$  from the salve boson study.

results discussed below. Figure 2 shows the critical temperature  $T_c$  of the  $d$ -wave superconducting phase for several values of  $U$ . This type of superconductivity is enhanced near the half-filled fermion system similarly as in the extended Hubbard model.<sup>25</sup> In agreement with our expectations, the Coulomb repulsion only weakly reduces  $T_c$  in a dilute fermion system. However, for  $\Delta_B = 0$  we notice a considerable reduction of  $T_c$  or even a disappearance of superconductivity for  $n - F = 1$  (total concentration is then  $n_{tot} = n_F + 2n_B = 2$ ) when  $U$  exceeds the critical Mott transition value  $U_{cr}$ . For such a strong potential  $U$  the  $d$ -wave superconducting phase is restricted to a narrower regime of the total concentration, such that there are no doubly occupied fermion states on a given lattice site (remember we are considering intersite Cooper pairs).

Figure 3 illustrates the effect of  $U$  on the extended  $s$ -wave phase. In a dilute regime we notice almost identical values of  $T_c$  for both the  $d$ - and extended  $s$ -wave superconducting phases. Also the influence of  $U$  is there very similar. A remarkable difference appears for  $\Delta_B = 0$  when the fermion system is near the half-filling  $n_F = 1$ . The critical temperature  $T_c$  of the  $s$ -wave phase is then 3 times smaller as compared to the  $d$ -wave phase. The system is thus less suscep-

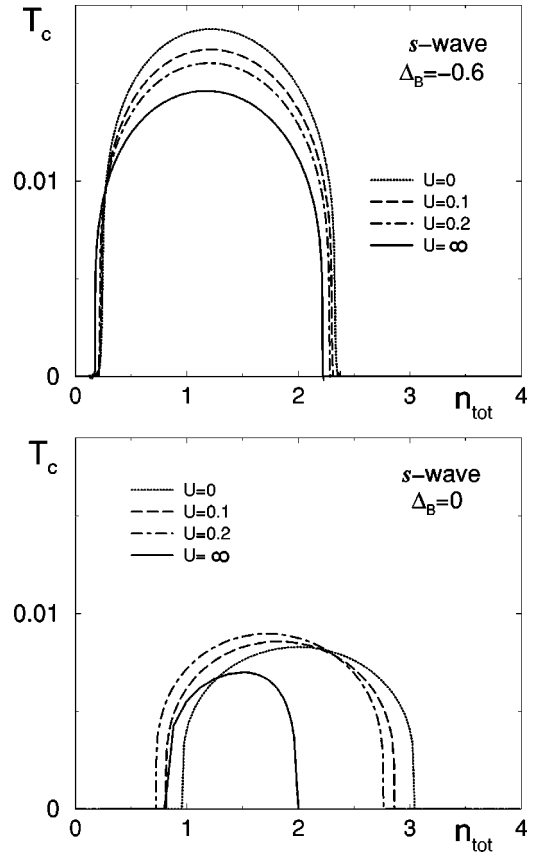


FIG. 3. Transition temperature  $T_c$  into the extended  $s$ -wave superconducting phase for several values of the on-site repulsion, as indicated. The top figure corresponds to  $\Delta_B = -0.6$  and the bottom one to  $\Delta_B = 0$ .

tible for the  $s$ -type pairing near  $n_F = 1$  (for  $\Delta_B = 0$  it corresponds to  $n_{tot} = 2$ ).

One notices also some “peculiar” behavior of  $T_c(n_{tot})$  for the extended  $s$ -wave phase generated by an increasing strength of  $U$ . With a small increase of  $U$  the whole diagram is somewhat shifted and simultaneously the optimal value of  $T_c$  slightly increases. This overall shift is caused by the Hartree term  $Un_F/2$  (see Sec. III) which effectively pulls up the fermion band with respect to the boson energy level. By comparing the curves corresponding to  $U = 0$  in the upper and bottom panels of Fig. 3 we realize that such a shift is responsible for enhancing the  $s$ -wave-type superconductivity, but only when  $U$  is safely smaller than  $D$ . A further increase of the Coulomb interaction  $U$  proves to be detrimental on superconductivity (independently of a symmetry of the order parameter) because the fermion subsystem is driven into the Mott insulating state.

To analyze in more detail the pronounced effect of the Coulomb interaction on superconductivity for the half-filled fermion system  $n_F = 1$  ( $n_{tot} = 2$ ) we show in Fig. 4 the dependence of  $T_c$  on  $U$ . The results have been obtained by means of the alloy analogy approximation mentioned in Sec. III and discussed earlier by the same author in Ref. 23. For the dim=2 tight-binding dispersion we determine the Mott transition at  $U_{cr} \approx 0.54$  in units of the initial fermion band. This value is probably underestimated. The most credible

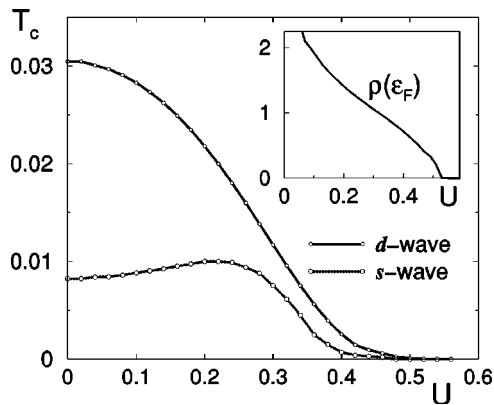


FIG. 4. Transition temperature  $T_c$  of the  $d$ - and the extended  $s$ -wave phases for the half-filled fermion system  $n_F=1$ . Both superconducting phases disappear when the Mott transition is approached. The inset shows the density of states at the Fermi energy for a normal phase obtained by the alloy analogy Approximation.

determination based on the dynamical mean-field theory usually yields  $U_{cr}$  larger than 1.<sup>26</sup> Nevertheless, the qualitative behavior presented in Fig. 4 remains valid. As we see by comparing to Figs. 2 and 3 the AAA treatment properly interpolates between the  $U=0$  and  $U=\infty$  limits.

## VII. CONCLUSIONS

Summarizing, we have investigated the anisotropic superconductivity within the boson-fermion model in the presence of the Coulomb repulsion between fermions.

(a) In a dilute regime of the fermion concentration the effect of the Coulomb repulsion proves to be rather weak. For both the  $d$ - and extended  $s$ -wave phases we observe up to a 25% reduction of the optimal  $T_c$  value when  $U \rightarrow \infty$ . Both anisotropic phases survive, even in the limit of infinitely strong Coulomb repulsions.

(b) In the nearly half-filled fermion system we observe an enhancement of the  $d$ -wave superconducting phase and a simultaneous suppression of the  $s$ -wave phase until the interaction  $U$  is small.

(c) Around the Mott transition  $U_{cr} \approx 0.54$  both phases are reduced to the concentration regime  $n_F < 1$ ,  $2n_B < 1$ . Still, the superconductivity is able to survive at sufficiently large hole concentrations  $h = 1 - n_F > 0$ . Such a case is relevant for a description of the HTSC materials and the boson-fermion model seems to be capable of reproducing qualitatively the phase diagrams known for these materials.

Among the problems which are not addressed in this paper there is a very intriguing question: what happens to the pseudogap of the normal phase (discussed earlier in the Refs. 8, 10, 11, 13, and 19 in the presence of Coulomb interactions? Consideration of this subject is in progress and the results shall be discussed elsewhere.

## ACKNOWLEDGMENTS

The author kindly acknowledges helpful discussions with J. Ranninger and K.I. Wysokiński. Partial support has been provided by the Polish Committee of Scientific Research under Project No. 2P03B 106 18.

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